

2,4-Octadienal

Inchi:	InChI=1S/C8H12O/c1-2-3-4-5-6-7-8-9/h4-8H,2-3H2,1H3/b5-4+,7-6+
InchiKey:	DVVATNQISMINCX-YTXXJHMSA-N
Formula:	C8H12O
SMILES:	CCCC=CC=CC=O
Mol. weight [g/mol]:	124.18

Physical Properties

Property code	Value	Unit	Source
gf	77.40	kJ/mol	Joback Method
hf	-59.59	kJ/mol	Joback Method
hfus	19.17	kJ/mol	Joback Method
hvap	40.04	kJ/mol	Joback Method
log10ws	-2.16		Crippen Method
logp	2.098		Crippen Method
mcvol	116.550	ml/mol	McGowan Method
pc	3059.17	kPa	Joback Method
rinpol	1124.00		NIST Webbook
rinpol	1116.00		NIST Webbook
rinpol	1113.00		NIST Webbook
tb	439.42	K	Joback Method
tc	627.33	K	Joback Method
tf	211.76	K	Joback Method
vc	0.461	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	225.21	J/mol×K	439.42	Joback Method
cpg	276.76	J/mol×K	596.01	Joback Method
cpg	267.58	J/mol×K	564.70	Joback Method
cpg	257.87	J/mol×K	533.38	Joback Method
cpg	247.60	J/mol×K	502.06	Joback Method
cpg	236.72	J/mol×K	470.74	Joback Method
cpg	285.43	J/mol×K	627.33	Joback Method

dvisc	0.0002188	Paxs	439.42	Joback Method
dvisc	0.0002838	Paxs	401.48	Joback Method
dvisc	0.0003886	Paxs	363.53	Joback Method
dvisc	0.0005725	Paxs	325.59	Joback Method
dvisc	0.0009343	Paxs	287.65	Joback Method
dvisc	0.0017693	Paxs	249.70	Joback Method
dvisc	0.0042123	Paxs	211.76	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R604430&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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